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Quantum Cellular Automata

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Research Summary

The Notre Dame group has developed a new paradigm for ultra-dense and ultra-fast information processing in nanoelectronic systems. These "Quantum Cellular Automata" (QCA's) are the first concrete proposal for a technology based on arrays of coupled quantum dots. The basic building block of these cellular arrays is the *Notre Dame Logic Cell*, as it has been called in the literature. The phenomenon of Coulomb exclusion, which is a synergistic interplay of quantum confinement and Coulomb interaction, leads to a bistable behavior of each cell which makes possible their use in large-scale cellular arrays. The physical interaction between neighboring cells has been exploited to implement logic functions. New functionality may be achieved in this fashion, and the Notre Dame group invented a versatile majority logic gate. In a series of papers, the feasibility of QCA wires, wire crossings, inverters, and Boolean logic gates was demonstrated. A major finding is that all logic functions may be integrated in a hierarchical fashion which allows the design of complicated QCA structures. The most complicated system which was simulated to date is a one-bit full adder consisting of some 200 cells. In addition to exploring these new concepts, efforts are under way to physically realize such structures both in semiconductor and metal systems. Extensive modelling work of semiconductor quantum dot structures has helped identify optimum design parameters for QCA experimental implementations. In the first year of this project, the experimental effort has laid the ground work for the study of Coulomb coupling in quantum dot structures. The newly acquired ultra-high resolution field emission scanning electron microscope was installed and used to examine nanostructures with a resolution of 1 nanometer. Coupled dot structures were fabricated in Gallium Arsenide heterostructures and await testing in the newly-established cryogenic measurement facility

Organization of the Report

Research Description

- **Bistability of Coulomb-coupled quantum dot cell.** For a family of cell designs, based on "quantum dot molecules" composed of near-by quantum dots, we demonstrated that Coulomb interaction produces a very nonlinear bistability in the charge distribution of the cell. The cell ground state is in one of two states depending on the electrostatic environment, which is in turn determined by neighboring cells. We introduced the concept of cell polarization to describe the possible alignment of charge within the cell.

- **QCA binary wires.** The intrinsic bistability of each cell coupled with the Coulomb interaction between cells causes a linear array of cells to align in the same polarization. The linear array thus acts as a binary wire, transmitting information from the driven end to the unconstrained end. We have explored the behavior of the wire for the entire parameter space of our model Hamiltonian. We found that the wire functioned well so long as the energetics of the Coulomb interaction dominated the kinetic energy which tends to cause the two-electron wavefunction to spread. The bistability of each cell in the wire also resulted in an insensitivity to geometrical variations and other parameter fluctuations from cell to cell.

- **QCA majority logic gate.** We designed the basic logical device in this architecture — the majority logic gate. Signals from three input wires converge on a single cell, from which the output emerges. The majority logic gate itself contains only two electrons and performs a logical function that would take many transistors to accomplish.

- **QCA inverter and wire crossing.** We devised a scheme for crossing two QCA wires in the plane by exploiting the symmetry of the charge distribution in the cells. This allows design of more complicated logical devices without the need to construct bridges for one QCA wire to cross another. A simple binary logical inverter device was also devised.

- **Hierarchical design of QCA circuits: the full adder.** We designed and simulated a single-bit full adder using QCA cells. The calculation involved self-consistently solving the Schrödinger equation for over 200 electrons. The Coulomb interaction between each pair of electrons was included. The results showed that the adder worked correctly for all possible inputs, and that hierarchical design rules are possible. Having developed the basic logical primitives, wires, inverters, majority gates, and wire crossings, design and layout can proceed without concern about spurious Coulomb interactions between various parts of the system. This is fundamentally due to the fact the cell has only a quadrupole moment with a rapidly decaying field strength.

- **QCA bistability implemented in metallic system.** The QCA systems we have considered so far were envisioned as being implemented in semiconductor quantum dots in which the total number of electrons could be made small and be well controlled. We have extended and generalized these ideas to cells composed of small metallic tunnel-junctions. In this case, each cell contains two *extra* electrons and the coupling between cells is capacitive (and therefore more controllable).

- **Time dependence of QCA devices.** By design, the exact time evolution of the QCA device after the inputs are switched is not crucial. The architecture works by mapping the ground state of the system, subject to the (newly imposed) boundary conditions, onto the solution of the logical or arithmetic problem. The details of how the system reaches that ground state, dissipating the switching energy, are not important. An exception to this occurs if the system dynamics are such

that the system becomes stuck in a metastable state and is unable to reach the new ground state in a reasonable time. In particular, this may occur in the situation of wire fan-out, where one signal is being spread to several different devices. To address this issue we have begun time-dependent calculations of the switching behavior of QCA devices. While preliminary results are encouraging, we have not completed this stage of our investigation.

- **Boundary Conditions for Quantum Devices with Exposed Surfaces.** We have developed a numerical technique for the simulation of the electrostatic potential and the electronic states in quantum device structures. Since we are particularly interested in quantum dots in the few electron regime, one of the main design strategies is to utilize semiconductor heterostructures with very shallow two-dimensional electron gases. Metallic gates on the semiconductor surface will then result in crisp confining potential landscapes. Since the electrons now are close to the surface, any surface charges will tend to alter the confining potentials. This poses challenges for the modelling of these structures since no simple boundary conditions for the potential on the surface are applicable. The usual Dirichlet and von Neumann boundary conditions, which are routinely employed for larger structures, are too simplistic in this case. In our modelling, therefore, we include both the semiconductor domain and the adjacent region of the dielectric (air or vacuum). The usual boundary conditions on the semiconductor surface are then replaced by matching conditions for the electrostatic potential and the dielectric flux. Any surface charges, such as the ones due to charged surface states, will lead to a discontinuity of the dielectric flux. We have developed an efficient numerical technique to solve for the electrostatic potential in the combined semiconductor - dielectric domains. Our approach is based on a coupled finite element method for the semiconductor domain and a boundary element method for the dielectric domain. The combined linear system of equations which has to be solved is only slightly larger than the one for the semiconductor alone.

- **Modelling of Quantum Dots in the Few Electron Regime.** Utilizing our numerical technique for the simulation of quantum device structures, we have studied field-confined quantum dots in the few electron regime. This numerical modelling will yield the design parameters for the experimental realization of QCA quantum dots cells. So far, we have explored the feasibility of several top-gate configurations and we have studied their capability of producing crisp confining potentials. The usual mode is to employ top gates with a negative bias, which repel the carriers in the two-dimensional electron gas underneath. Quantum wires and quantum dots are realized in the areas below metal-free regions on the surface, which expose the semiconductor to the ambient dielectric. Our modelling shows that for typical dimensions and structural parameters, it will be very difficult to use negative gate biases to tune quantum dots which are occupied by a small number of electrons. Even for extremely small separations of the 2DEG from the surface, say 40 nm or so, the confining electrostatic potential is still quite gradual. It will also be very difficult to realize top metal gates with openings which are on the order of only a few tens of nanometers. In addition, the geometrical features of the metal opening are several times larger than the induced dot underneath. This will make it very hard, if not impossible, to fabricate a QCA cell, which contains several closely-spaced dots, by utilizing negative top-gate biasing. An alternate approach is to use positive top-gate biasing. In this scheme, one starts out with a structure which does not possess a two-dimensional electron gas without biasing. A positive bias applied to the metal on the top surface may then induce electrons underneath. Our modelling of this accumulation mode shows that geometrical considerations allow the realization of closely-spaced dots. However, the positive bias required is so large that the structure becomes leaky (between top metal and 2DEG).

The most promising approach, which we were able to identify based on our modelling work, is a combined depletion mode (negative top-gate bias) and accumulation mode (positive top-gate bias). We envision a top-gate geometry which consists of a rather large opening (negative bias) in which several metal dots (positive bias) are placed. The negative gate just barely depletes the 2DEG, and the carriers may be brought back with a rather small positive bias. We are hopeful that a QCA cell may be realized by this combined biasing approach. The opening in the negative gate will define a whole cell and the dots in each cell will be induced by separate positively-biased gates placed inside the opening. The modelling of experimental test structures is under way.

• **QCA Realization in III-V's.** Graduate student Greg Bazán has made significant progress over the last year toward demonstration of Coulomb coupling in III-V material. He has designed a set of molecular beam epitaxy layers provided by Dr. J. Furdyna at Notre Dame, improved the operation of the Heliox cryostat dewar, and fabricated first devices to be tested soon. Figure 1 shows SEM micrographs of a set of two "dots" fabricated on a 2DEG designed to detect the presence of one electron per dot. The two quantum dots are at the top and bottom of the center bounded at the top by TD, F, QG, and R, and at the bottom by JN, P, QG, and H. In the configuration shown, a wide barrier has been built between the quantum dots so that the dots can be tested independently. In future iterations, this barrier will be made thinner or replaced by a split gate so that the effects of coupling can be investigated.

By biasing these Schottky contacts correctly, the dot areas can be squeezed so that the energy well of the dot can support a varying electron population. We will first discuss the top quantum dot. Electrons are brought into, or pushed off of, the dot through split-gates R-TD and F-TD by ohmic contacts SE. The presence of extra electronic charge on the dot is detected through biasing split gate B-TD below the first conductance step. The conductance there is small, due only to thermal broadening of the Fermi level, but will be noticeably modified by the presence a single extra electron. Therefore, we see that the structure consists of two dots and two detectors. By the presence of a backgating layer structure, we can independently change the electron population and the dot size, while biasing split gates to place or remove single electrons from a dot and observing the effect on the adjacent dot through its detector. This is a very complicated experiment, and although much has been accomplished so far, significant groundwork is still required before we can test the entire functionality of the structure.

• **QCA Realization in Metals.** The identical functionality as that described above can be performed in an entirely metal/insulator system using single electron charging phenomena. Graduate Student Xiaokang Huang has undertaken to demonstrate Coulomb coupling using tunnel junctions fabricated by the technique of shadow evaporation[1] pioneered by Dolan.

Lafarge *et al.*[2] have shown that it is possible to detect, by capacitive coupling only, a single electron tunneling onto a metal island. Using shadow evaporation technology, we have designed a four-dot QCA cell, as suggested by C. Lent and shown in Fig. 2. C1 and similar structures repre-

1. G. J. Dolan, *Phys. Rev. Lett.* **31**, 109 (1977).
2. P. Lafarge, H. Pothier, E. R. Williams, D. Esteve, C. Urbina, and M. H. Bevoret, *Phys. B- Condensed Matter* **85**, 327 (1991).

sent tunnel junctions with all metal adjacent to "a" representing a "dot" capacitively coupled

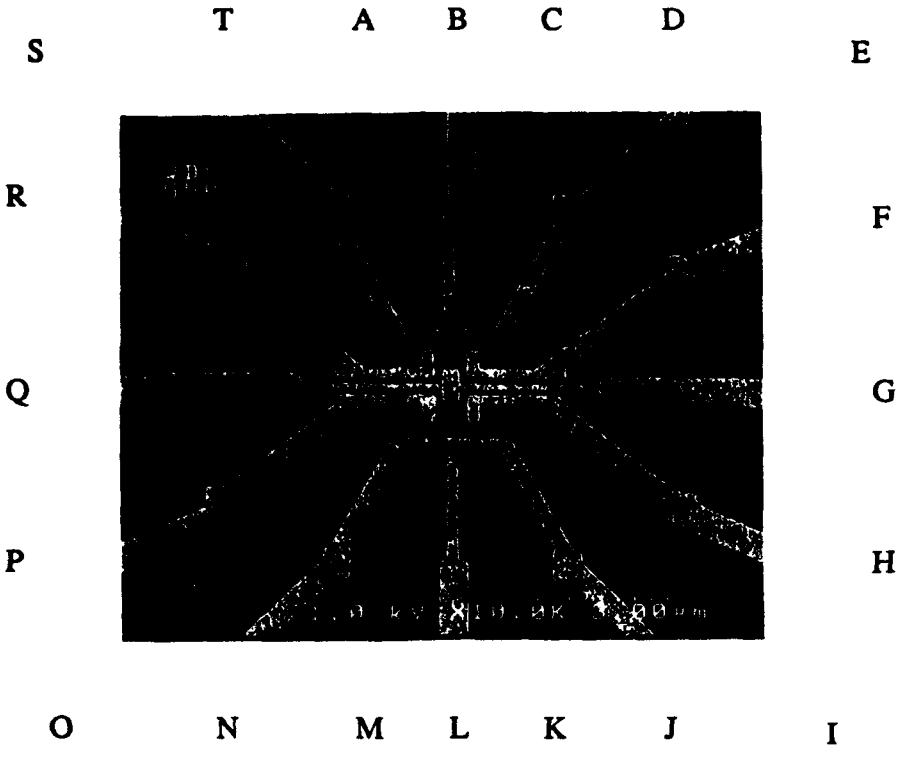

Figure 1. Electron micrograph of devices fabricated by EBL for the purpose of testing Coulomb coupling between quantum dots. All metal in this photo are Schottky layers for the creation of energy barriers in the 2DEG.

(through capacitor Cc) to the metal at "c", another quantum dot.

Figure 3 shows a plot of the physical layout of the complete cell. All structures are metal, except for thin AlO_x layers acting as tunnel barriers at the overlapping points, indicated by the shaded regions. As single electrons tunnel onto a metal island, e.g. at I1, adjacent metal lines at I1 capacitively couple the electric field to I3 and affect the ability for an electron to tunnel onto I3. Electrodes 2,4,7, and 9 can be used to bias the dots, and electrodes 3 and 8 will be used to screen the bias fields from each other.

Figure 4 shows a cross-section of a thin layer of PMMA over a thick layer of PMMA/MAA copolymer which, after EBL exposure and developing, has resulted in an extreme undercut profile allowing evaporation of metal at relatively large angles- as much as 6 degrees off vertical. At the top,the thin opening is a faithful representation of the EBL exposure in PMMA, whereas the PMMA/MAA developed more quickly creating the undercut. Visible is the aluminum line evaporated through the slit at the top and resting on the surface of the wafer off from the vertical. This

technique allows us to evaporate a line, oxidize it *in situ*, and then, after tilting the sample, evaporate another line perpendicular to it so that an overlap is achieved resulting in a single electron tunnel junction. Figure 5 shows perpendicular aluminum lines overlapping in a region approximately 50 by 80 nm^2. So far, complete structures have been fabricated, but accurate control of tunneling resistance has not been achieved.

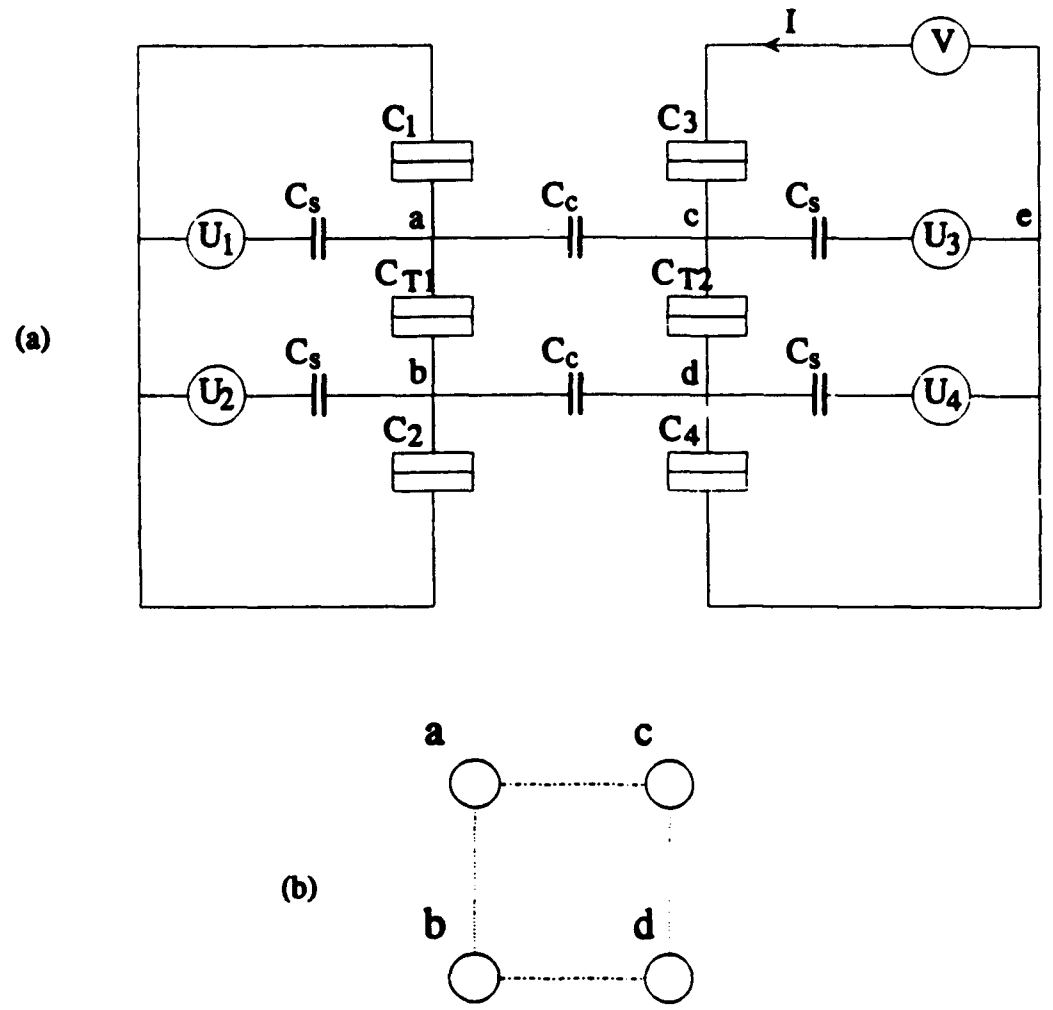

Figure 2. (a) Schematic of the prototype QCA consisting of 4 single electron "dots." (b) Diagram of the QCA cell formed by (a).

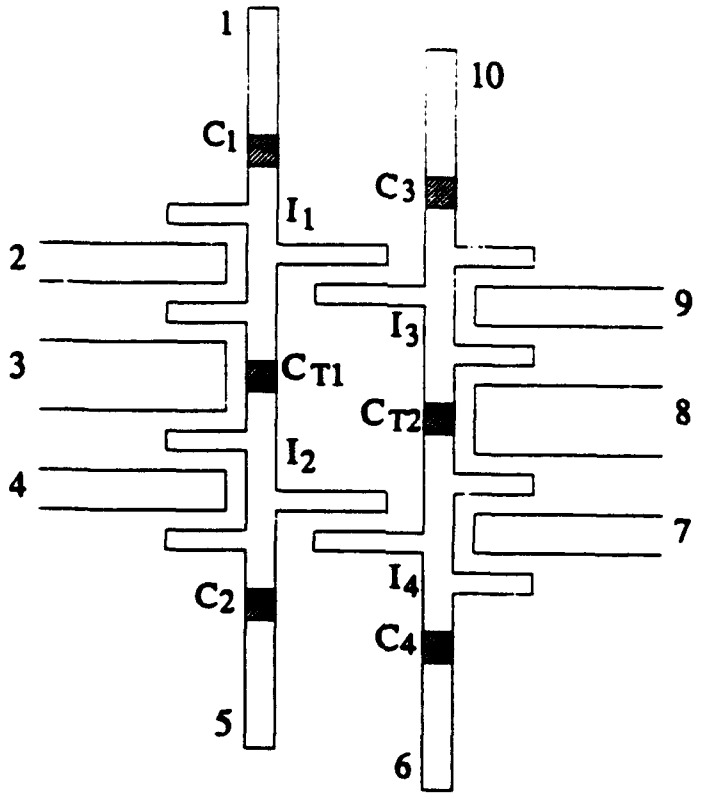

Figure 3. Physical layout of the prototype QCA shown in Fig. 5.

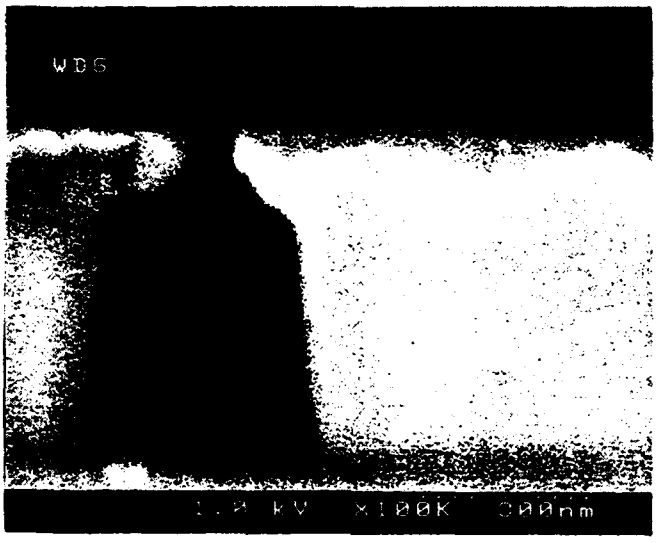

Figure 4. FESEM micrograph of cross-sectioned double resist layers used for shadow evaporation. The metal line evaporated at 6 degrees off normal is visible on the surface of the wafer.

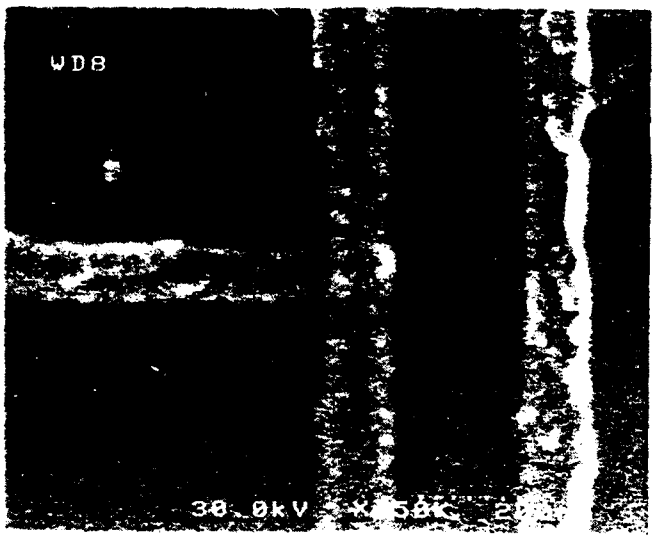

Figure 5. FESEM micrograph of tunnel junction formed by the Dolan bridge technique. A second, unused, vertical line exists due to the double, angled shadow evaporation. The aluminum has been oxidized between evaporations.

Journal Publications

Craig S. Lent, P. Douglas Tougaw, Wolfgang Porod, and Gary H. Bernstein, "Quantum Cellular Automata," *Nanotechnology* **4**, 49-57 (1993).

Craig S. Lent, P. Douglas Tougaw, and Wolfgang Porod, "Bistable Saturation in Coupled Quantum Dots for Quantum Cellular Automata," *Applied Physics Letters* **62**, 714 (1993).

X. Huang, G. Bazán, G. H. Bernstein, "New Technique for Computation and Challenges for Electron Beam Lithography," *Journal of Vacuum Science and Technology B*, **11**(6), 2565-2569 (1993).

Craig S. Lent and P. Douglas Tougaw, "Lines of interacting quantum-dot cells: a binary wire," *Journal of Applied Physics*, **74**, 6227 (1993).

P. Douglas Tougaw, Craig S. Lent, and Wolfgang Porod, "Bistable saturation in coupled quantum-dot cells," *Journal of Applied Physics* **74**, 3558-3566 (1993).

Craig S. Lent and P. Douglas Tougaw, "Bistable saturation due to single electron charging in rings of tunnel junctions," *Journal of Applied Physics* **75**, 4077-4080 (1994).

P. Douglas Tougaw and Craig S. Lent, "Logical devices implemented using quantum cellular automata," *Journal of Applied Physics* **75**, 1818-1825 (1994).

Minhan Chen, Wolfgang Porod, and David J. Kirkner, "A Coupled Finite Element/Boundary Element Method for Semiconductor Quantum Devices with Exposed Surfaces," Journal of Applied Physics **75**, 2545-2554 (1994).

Conference Publications and Presentations

Gary H. Bernstein, Xiaokang Huang, Greg Bazán, Davide A. Hill, Craig S. Lent, and Wolfgang Porod, "New Technique for Computation and Challenges for Electron Beam Lithography," poster presented at the *Three-Beams Conference*, San Diego, California, June 1993.

Craig S. Lent, Wolfgang Porod, and P. Douglas Tougaw, **(Invited)**, "Quantum Simulation of Several-Particle Systems," presented at the *Workshop on Combined Self-Consistent Particle Transport Simulation and Full Wave Dynamic Field Simulation for Monolithic Solid State Device and Circuit Calculations of the IEEE Microwave Theory and Techniques Symposium*, Atlanta, Georgia, June 1993.

Minhan Chen, Wolfgang Porod, and David J. Kirkner, "Boundary Conditions for Quantum Devices with Exposed Surfaces," *Proceedings of the International Workshop on Computational Electronics*, C. Snowden and M. Howes, eds., pp. 255 - 259; presented at the *International Workshop on Computational Electronics*, Leeds, England, August 1993.

Craig S. Lent, Wolfgang Porod, and P. Douglas Tougaw, "Quantum Simulation of Several-Particle Systems," *Proceedings of the "International Workshop on Computational Electronics*, C. Snowden and M. Howes, eds., pp. 303 - 307; presented at the *International Workshop on Computational Electronics*, Leeds, England, August 1993.

C. S. Lent, P. D. Tougaw, W. Porod, and G. H. Bernstein, **(Invited)**, "Quantum Cellular Automata," presented at the *Midwest Solid State Theory Symposium*, Detroit, Michigan, October, 1993.

Craig S. Lent, Wolfgang Porod, and Gary H. Bernstein, **(Invited)**, "Quantum Cellular Automata," presented at the 1993 ARPA ULTRA review meeting, Santa Fe, New Mexico, October 1993.

Craig S. Lent, **(Invited)**, "Quantum Cellular Automata," *International Conference on Advanced Microelectronic Devices and Processing*, Sendai, Japan, March 1994.

Craig S. Lent, P. Douglas Tougaw, and Wolfgang Porod, "Quantum Cellular Automata," abstract published in the *Bulletin of the APS*, Vol. 39, No. 1, p. 799, March 1994; presented at the *1994 March Meeting of the American Physical Society*, Pittsburgh, Pennsylvania, March 1994.

P. Douglas Tougaw and Craig S. Lent, "Dynamics of a linear array of coupled quantum-dot cells," *American Physical Society March Meeting*, Pittsburgh, Pennsylvania, 1994.

Minhan Chen and Wolfgang Porod, "Numerical simulation of electron confinement in quantum dot structures," abstract published in the *Bulletin of the APS*, Vol. 39, No. 1, pp. 800 - 801, March 1994; presented at the *1994 March Meeting of the American Physical Society*, Pittsburgh, Pennsylvania, March 1994.

B. Campbell, G. H. Bernstein X. Huang, and G. Bazán, "A Novel Method for Producing Nanostructures in Silicon Inversion Layers," presented at the *March Meeting of the American Physical Society*, Pittsburgh, Pennsylvania, March 1994.

G. Bazán and G. H. Bernstein, "Nanolithography over Very Large Scan Fields," poster presented at *Great Lakes Symposium on VLSI*, Notre Dame, Indiana, March, 1994.

X. Huang, G. Bazán, and G. H. Bernstein, "Proximity Effects in Ultradense Patterns Exposed by Electron Beam Lithography," poster presented at *Great Lakes Symposium on VLSI*, Notre

Dame, Indiana, March, 1994.

Craig S. Lent, **(Invited)**, "Quantum Cellular Automata," presented at the *Engineering Foundation Conference on Surfaces and Interfaces in Mesoscopic Devices*, Kona, Hawaii, April 1994

Minhan Chen and Wolfgang Porod, "Numerical simulation of electron confinement in quantum dot structures," presented at the *Engineering Foundation Conference on Surfaces and Interfaces in Mesoscopic Devices*, Kona, Hawaii, April 1994.

Craig S. Lent, Manhua Leng, and P. Douglas Tougaw, **(Invited)**, "Quantum Device Modeling," presented at the *Third International Workshop on Computational Electronics*, Portland, Oregon, May 1994.

P. Douglas Tougaw and Craig S. Lent, "Dynamic Behavior of Coupled Quantum Dot Cells," presented at the *Third International Workshop on Computational Electronics*, Portland, Oregon, May 1994.

Minhan Chen and Wolfgang Porod, "Numerical Simulation of the Effect of Surface Charges on Electron Confinement in Quantum Dot Structures," presented at the *Third International Workshop on Computational Electronics*, Portland, Oregon, May 1994.

Invited Seminars

"Quantum Cellular Automata," Craig S. Lent, seminar presented at Wright Laboratories, Wright-Patterson AFB, Dayton Ohio, September 1993.

"Quantum Cellular Automata," Craig S. Lent, seminar presented at the Department of Electrical Engineering, University of Maryland, College Park, Maryland, October 1993.

"Quantum Dots Coupled in a Cellular Automata Architecture," Craig S. Lent, seminar presented at the Department of Physics and Astronomy, Michigan State University, East Lansing, Michigan, January 1994.

"Quantum Cellular Automata," Wolfgang Porod, seminar presented at Sandia National Laboratories, Albuquerque, New Mexico, February 1994.

"Quantum Cellular Automata," Craig S. Lent, colloquium presented at Indiana University-Purdue University, Indianapolis, April, 1994.

"Quantum Device Fabrication at Notre Dame," Gary H. Bernstein, seminar presented at Motorola, Inc., Tempe, Arizona, June 1994.

Honors, Awards, and Appointments

Wolfgang Porod served on the Advisory Committee of the *Second International Workshop on Computational Electronics*, Leeds, England, August 1993.

Wolfgang Porod was a member of the Technical Program Committee of the *Conference on Neural Networks and Artificial Intelligence* of the *SPIE International Symposium on Substance Identification Technologies*, Innsbruck, Austria, 4 - 8 October 1993.

Wolfgang Porod was a member of the Review Team for the *Electrical and Computer Engineering Graduate Program Review*, The University of New Mexico, Albuquerque, February 1994.

Gary H. Bernstein was a Session Chair at the *March Meeting of the American Physical Society*, Pittsburgh, Pennsylvania, March 1994.

Wolfgang Porod was a member of the Technical Program Committee of the *Third International Workshop on Computational Electronics*, Portland, Oregon, May 1994.

Gary H. Bernstein was a member of the Technical Program Committee and Session Chair at *The 38th International Symposium on Electron, Ion and Photon Beams*, New Orleans, Louisiana, May 1994.

APPENDIX: Coverpages of Reprints

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Quantum cellular automata

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Abstract. We formulate a new paradigm for computing with cellular automata (CAs) composed of arrays of quantum devices—quantum cellular automata. Computing in such a paradigm is *edge driven*. Input, output, and power are delivered at the edge of the CA array only; no direct flow of information or energy to internal cells is required. Computing in this paradigm is also *computing with the ground state*. The architecture is so designed that the ground-state configuration of the array, subject to boundary conditions determined by the input, yields the computational result. We propose a *specific realization* of these ideas using two-electron cells composed of quantum dots, which is within the reach of current fabrication technology. The charge density in the cell is very highly polarized (aligned) along one of the two cell axes, suggestive of a two-state CA. The polarization of one cell induces a polarization in a neighboring cell through the Coulomb interaction in a very non-linear fashion. Quantum cellular automata can perform useful computing. We show that AND gates, OR gates, and inverters can be constructed and interconnected.

1. Introduction

The continual down-scaling of device dimensions in microelectronics technology has led to faster devices and denser circuit arrays with obvious benefits to chip performance. Dramatic as they have been, these changes have been evolutionary in nature in that even the most advanced chips use the same paradigms for computing as their more primitive ancestors. There is now much expectation that the availability of very dense device arrays might lead to new paradigms for information processing based on locally-interconnected architectures such as cellular automata (CA) and cellular neural networks [1].

There has also been considerable interest in quantum mesoscopic structures for their possible application as devices [2]. Much has been learned about the behavior of electrons flowing through very small structures in semiconductors. Various investigators have pointed out the natural link between mesoscopic quantum systems and cellular automata architectures [3–5]. Because quantum structures are necessarily so small, it is difficult to conceive of a regime in which a single quantum device could drive many other devices in subsequent stages [6]. Furthermore, the capacitance of ultra-small wires forming the connections to each device would tend to dominate the behavior of an assembly of quantum devices. For these reasons locally interconnected structures such as cellular neural networks and CAs may provide the natural architecture for quantum devices.

We focus here on the idea of employing CA architectures which are compatible with nanometer-scale quantum devices—thus, *quantum cellular automata* (QCA). A QCA would consist of an array of quantum device cells in a locally-interconnected architecture. The cell state becomes identified with the quantum state of the mesoscopic device. Two-state CAs are attractive because they naturally admit to encoding binary information. For a two-state QCA, each cell should have two stable quantum states. The state of a given cell should influence the state of the neighboring cells. Two ingredients are essential then: (1) the bistability of the cell, and (2) coupling to neighboring cells.

We propose a cell which is composed of coupled quantum dots occupied by two electrons [7]. The requisite bistability is accomplished through the interaction of quantum confinement effects, the Coulomb interaction between the two electrons, and the quantization of charge [8]. The intercellular interaction is provided by the Coulomb repulsion between electrons in different cells. We analyze this cell and the interactions between neighboring cells in section 2.

In section 3 we propose a new paradigm for how computation could be performed with an array of quantum devices. Because no direct connections can be made to interior cells, information or *energy* can enter the array only from the edges. *Edge-driven computation* imposes further constraints on the nature of the computing process [9]. The lack of direct connections to the interior cells also means that no mechanism exists for keeping the array away from its equilibrium ground-state configuration. We are therefore led to use the ground state of the array to do the computation. *Computing with the ground state* means that the physics of the array must

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Bistable saturation in coupled quantum dots for quantum cellular automata

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A simple model quantum dot cell containing two electrons is analyzed as a candidate for quantum cellular automata implementations. The cell has eigenstates whose charge density is strongly aligned along one of two directions. In the presence of the electrostatic perturbation due to a neighboring cell, the ground state is nearly completely aligned (polarized) in one direction only. The polarization is a highly nonlinear function of the perturbing electrostatic fields and shows the strong bistable saturation important for cellular automation function.

Nanoscale quantum structures with potential device applications have been an active area of exploration for several years. A frequent criticism[1] of many of these structures is the absence of the saturating behavior which forces conventional transistor elements into one of two stable states, "on" or "off." Such bistable saturation is important to keep device performance robust in the presence of physical inhomogeneities and noise.[2]

The possibility of realizing cellular automata (CA) with regular arrays of quantum dots has been suggested by Bate and others.[3] In one example, the necessary nonlinear response of each dot is the result of resonant tunneling through the dot.[4] We focus on a different paradigm in which each cell of the CA is composed of groups of coupled quantum dots. The confining potentials are such that electrons can tunnel between dots in the same cell but not between different cells. Quantum mechanics and the Coulomb interaction in each cell determine the possible cell states. The Coulomb interaction between electrons in different cells provides a local intercellular coupling mechanism. The nonlinear response of the cell to its electrostatic environment must be a feature of the internal cell dynamics. Recent success in fabricating arrays of very small quantum dots with one or two electrons per dot[5] prompts us to investigate possible few-electron coupled-dot cell geometries which provides the sort of bistable saturation so desirable. In this letter, we analyze a possible cell geometry with two electrons in the cell. We show that quantum confinement and the intracellular Coulomb interaction together yield the nonlinear saturation behavior which is essential.

We examine a simple nanostructure model cell containing five coupled quantum dots. The model cell is shown schematically in Fig. 1. It consists of a central site and four neighboring sites. Tunneling is possible both between the outer sites and the central site, and between adjacent outer sites. We first consider such a cell holding two electrons (the contrasting case of single and triple cell occupancy is discussed below). We show below that the Coulomb repulsion between the two electrons causes the ground state of the system to be one in which the electrons occupy antipodal sites.

We model the cell using a Hubbard-type Hamiltonian with Coulomb repulsion. The Hamiltonian for a single isolated cell can be written,

$$H_0^{\text{cell}} = \sum_{i,\sigma} E_0 n_{i,\sigma} + \sum_{i,j,\sigma} t_{i,j}(a_{i,\sigma}^{\dagger} a_{j,\sigma} + a_{j,\sigma}^{\dagger} a_{i,\sigma}) + \sum_{i} E_Q n_{i,\uparrow} n_{i,\downarrow} + \sum_{i>j,\sigma,\sigma'} V_Q \frac{n_{i,\sigma} n_{j,\sigma'}}{|r_i - r_j|}, \quad (1)$$

where the number operator $n_{i,\sigma} = a_{i,\sigma}^{\dagger} a_{i,\sigma}$ and the operator $a_{i,\sigma}^{\dagger}$ creates an electron at site i with spin σ. The cell parameters which define the Hamiltonian are then the on-site energy, E_0, the tunneling energies, $t_{i,j}$, and the on-site Coulomb charging energy, E_Q. The parameter V_Q is determined by fundamental constants and the dielectric constant of the material in which the dots are formed. A fixed positive charge $\tilde{\rho}$ is assumed at each site sufficient to maintain overall cell charge neutrality. For an isolated cell, this only renormalizes E_0, but it is important in calculating the interaction between cells as is done below.

For the numerical results we discuss here we choose parameters based on a simple, experimentally accessible model. We consider a cell in a semiconductor with $m^* = 0.067 m_0$, which is composed of circular quantum dots of diameter $D = 10$ nm. The near-neighbor distance between the cells is 20 nm. The dielectric constant for the semiconductor is 10. We take $t = 0.3$ meV for coupling to the center site and $t = 0.03$ meV for coupling between outer dots. These tunneling energies can be varied greatly by adjusting the potential barriers between dots. We take $E_Q = V_Q/(D/3)$. We will assume here that the two electrons in the cell have antiparallel spins. The parallel spin case yields results which are qualitatively very similar.

The eigenstates of the Hamiltonian [Eq. (1)] can now be calculated for this specific choice of cell parameters. The Hamiltonian is diagonalized directly in the basis of few-electron states. From the two-electron wave function we calculate the single particle density at each site, ρ_i by find-

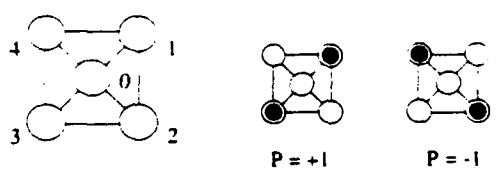

FIG. 1. The quantum cell consisting of five quantum dots which are occupied by two electrons. The mutual Coulomb repulsion between the electrons results in bistability between the $P = +1$ and $P = -1$ states.

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New technique for computation and challenges for electron-beam lithography

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In this article, the basic concepts of our recently proposed computing architecture based on Coulomb coupling of nanofabricated structures, called quantum cellular automata (QCA) are reviewed and fabrication issues critical to the new technology are discussed. The QCA fabrication will require an extremely high level of lithographic control. To this end, the proximity effects in making very high density patterns with poly(methylmethacrylate) (PMMA) and electron-beam lithography have been experimentally investigated. A triple Gaussian model was used to simulate the experimental data. By using a 50 keV electron beam, sub-40 nm pitch gratings, double lines, and dot grids were successfully fabricated on Si and SiO_2/Si bulk wafers with single-level PMMA and lift-off.

I. INTRODUCTION

High density patterns are very important for such structures as quantum devices and high speed photodetectors,[1] as well as studies of basic quantum phenomena, such as current drag.[2] Recently, we proposed a new paradigm for computing with cellular automata (CA) composed of arrays of quantum dots arranged into separate cells of several dots.[3,4] We call this new architecture "quantum cellular automata" (QCA). Our calculations show that the dots, which are fundamental to the new architecture (discussed below), must be as small as 10–15 nm in diameter on a pitch of 15–30 nm with intracell variations of at most 5%–10% over a few micron area. This implies that electron-beam lithography (EBL) to be used in the fabrication will be put to a serious test. Although Allee *et al.*[5,6] have directly patterned 15 nm gratings on SiO_2/Si with EB irradiation, lift-off with poly(methylmethacrylate) (PMMA) is still one of the most common techniques used in pattern transfer. The latter has so far produced results in the 40–50 nm pitch range.[1] In this size regime, pitch is limited by the strength of PMMA and proximity effects during exposure.

Proximity effects result from the distributions of injected and scattered electrons in the resist. Because of the distributions, the resist which is not directly addressed by the primary EB will also be exposed. The electron distributions in resist have been discussed in many papers,[7–9] and a triple Gaussian model[8–10] was used in modeling the distributions. The triple Gaussian model is

$$f(r)=\frac{1}{\pi(1+\eta+\eta')}\left[\frac{1}{\alpha^2}\exp\left(-\frac{r^2}{\alpha^2}\right)+\frac{\eta}{\beta^2}\exp\left(-\frac{r^2}{\beta^2}\right)+\frac{\eta'}{\gamma^2}\exp\left(-\frac{r^2}{\gamma^2}\right)\right]. \quad (1)$$

The first term includes the distributions of the primary electron beam and forward scattered electrons. The width of the term α ranges from a few nm to tens of nm, which depends on the beam size and energy, and the resist. The second term only includes the backscattered electrons from the substrate. The width of the distribution of backscattered electrons β is a few microns and depends on beam energies and types of substrates. The higher the beam energy, the wider the distribution.[11] The third term, the "broad range electrons,"[10] describes the behavior of all other electrons that are not included in the first two terms.[8,9] Its width γ is a few hundreds of nm. Here, η and η' are the ratios of the exposures of the β and γ term to the forward exposure, respectively.

Because of their distributions, different electrons result in proximity effects in different ranges. Although there are many papers that have investigated the proximity effects in EBL[8,9,12] and many methods for computer-aided proximity effect corrections during EBL have been developed,[13,14] the feature sizes and spacing in most of the published work are in the half- or quarter-micron regime, which is important in ultra-large scale integration (ULSI) circuit fabrication. Since large throughput is required in manufacturing, low beam energy (20 keV) and large currents are used in industrial EBL. In that case, backscattered electrons can dominate the proximity effects. However, for making very high density patterns that approach the spatial density limit of EBL, high beam energy (50 keV or higher), and small beam size (smaller than 10 nm) are usually used. In applications of nanolithography for quantum devices, pattern sizes are usually very small compared to those of ULSI. Therefore, the proximity effects from forward scattered electrons and secondary electrons become more pronounced.[10]

In this article, we discuss the basic properties and requirements of the QCA architecture. Toward the achievement of the required size scales, we report an experimental investigation of proximity effects for lines with pitch down to 50 nm. A triple Gaussian model is used in the theoretical simulation of the experimental results. The purpose of discussing the proximity effects is not directly to make proximity corrections in processing, but to understand and overcome the difficulties in making high density patterns. A spatial density limit in gratings caused by the proximity effects in PMMA is also determined. We studied the proximity effects in gratings rather than in arrays of dots (which will be more typical of the QCA work to be done)

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Lines of interacting quantum-dot cells: A binary wire

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The behavior of linear arrays of cells composed of quantum dots is examined. Each cell holds two electrons and interacts Coulombically with neighboring cells. The electrons in the cell tend to align along one of two axes resulting in a cell "polarization" which can be used to encode binary information. The ground-state polarization of a cell is a highly nonlinear function of the polarization of its neighbors. The resulting bistable saturation can be used to transmit binary information along the line of cells, thus forming a binary wire.

I. INTRODUCTION

Many investigators have noted the connection between quantum devices and locally interconnected architectures.[1] The small currents and charges inherent in quantum devices are poorly suited for driving large numbers of devices, particularly conventional devices. Requiring that a quantum device interact only with its neighbors is much more promising. Despite the appeal of this synthesis, few proposals including both a specification of the component quantum devices and the coupling between them have appeared.[2]

Recently, a specific proposal for a quantum cellular automata (QCA) implementation has been made by the authors *et al.*[3,4] The scheme is based on a quantum cell composed of several quantum dots and containing two electrons. Coulomb repulsion between the electrons causes the charge in the cell to align along one of two directions. These two alignment states, "polarizations," are used to encode binary information. The Coulomb coupling of the charge distribution in one cell to the charge in neighboring cells provides a physics-based local coupling between cells. The coupling leads to a highly bistable saturation behavior in the polarization, avoiding some of the criticisms of usual quantum interference-based device characteristics.[5] Specific arrangements of cells which can function as AND and OR gates have been proposed.

In this article we examine in detail the linear arrays of such quantum-dot cells which form the "wires" in the QCA scheme proposed. In the following section we review the physics of the basic cell and the model proposed in Ref. 3. Section III presents the theoretical machinery, a Hartree self-consistency scheme, which we use to examine arrays of cells. Section IV contains the examination of the behavior of a linear array of cells. We show that for a large range of physical parameters, the linear array behaves as a binary wire. Section V contains a discussion of the results.

II. COUPLED QUANTUM CELLS

The quantum-dot cell is shown schematically in Fig. 1(a). It consists of four quantum dots on the corners of a square and one central dot.[6] The cell is occupied by two electrons.[7,8] Tunneling occurs between near neighbors and next-nearest neighbors but the barriers between cells are assumed sufficient to completely suppress electron tunneling between cells. We treat the quantum dots in the site representation, ignoring any degrees of freedom within the dot.

A. Cell polarization

The Coulomb interaction causes the two electrons to tend to occupy antipodal sites. The two-electron ground state may then consist of the electrons aligned along one of two perpendicular axes as shown in Fig. 1(b). We define a quantity called the cell polarization which measures the extent to which the charge is aligned along one of these two axes. We denote the single-particle density at site i as ρ_i. The polarization is then defined as

$$P \equiv \frac{(\rho_1+\rho_3)-(\rho_2+\rho_4)}{\rho_0+\rho_1+\rho_2+\rho_3+\rho_4}. \tag{1}$$

If the two electrons are entirely localized in sites 1 and 3, then the polarization $P=1$. If the electrons are on sites 2 and 4, $P=-1$. An isolated cell would have a ground state which is a linear combination of these two polarizations, hence a net polarization of zero.[9]

B. The cell Hamiltonian

We construct a simple model of the cell using a tight-binding Hubbard-type Hamiltonian. For an isolated cell, the Hamiltonian can be written

$$H_0^{\text{cell}} = \sum_{i,\sigma} E_0 n_{i,\sigma} + \sum_{i>j,\sigma} t_{i,j}(a_{i,\sigma}^{\dagger} a_{j,\sigma} + a_{j,\sigma}^{\dagger} a_{i,\sigma}) + \sum_{i} E_Q n_{i,\uparrow} n_{i,\downarrow} + \sum_{i>j,\sigma,\sigma'} V_Q \frac{n_{i,\sigma} n_{j,\sigma'}}{|\mathbf{R}_i - \mathbf{R}_j|}. \tag{2}$$

Here $a_{i,\sigma}$ is the annihilation operator which destroys a particle at site i ($i=0,1,2,3,4$) with spin σ. The number operator for site i and spin σ is represented by $n_{i,\sigma}$. The on-site energy for each dot is E_0, the coupling between the ith and jth dot is $t_{i,j}$, and the on-site charging energy (the Coulomb cost for two electrons of opposite spin occupying the same dot) is E_Q. The last term in the Hamiltonian represents the Coulombic potential energy for two electrons located at sites i and j at positions $\mathbf{R}_i$ and $\mathbf{R}_j$.

For our "standard cell," on which most of the numerical results reported here are based, we obtain the values of the parameters in the Hamiltonian from a simple, experi-

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Bistable saturation in coupled quantum-dot cells

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Model quantum dot cells are investigated as potential building blocks for quantum cellular automata architectures. Each cell holds a few electrons and interacts Coulombically with nearby cells. In acceptable cell designs, the charge density tends to align along one of two cell axes. Thus, a cell "polarization," which can be used to encode binary information, is defined. The polarization of a cell is affected in a very nonlinear manner by the polarization of its neighbors. This interaction is quantified by calculating a cell–cell response function. Effects of nonzero temperature on the response of a model cell are investigated. The effects of multiple neighbors on a cell are examined and programmable logic gate structures based on these ideas are discussed.

I. INTRODUCTION

For many years, the size of microelectronic devices has been shrinking, and this has led to faster, denser circuits. Despite these improvements, the basic computing paradigm has remained virtually unchanged because device operation has been largely unaltered, apart from rescaling. There is now much interest in extremely dense device arrays forming locally interconnected architectures like cellular automata (CA)[1] and cellular neural networks.[2] Such architectures could lead to changes in device structure of a less evolutionary and more revolutionary nature.

At the same time, many researchers have been investigating ways to use quantum structures as electronic devices. In the course of such research, a great deal has been learned about the behavior of electrons in very small structures. Because of the size of the structures involved, an outstanding difficulty is providing a scheme in which one of these quantum devices, which typically carry nanoamperes of current, could be used to drive several other similar devices. In addition, the capacitance of the wires needed to interconnect such structures would tend to dominate their behavior. Therefore, locally connected architectures like CA's may be an attractive paradigm for implementing quantum device architectures.[3]

CA architectures composed of nanometer-scaled quantum devices that are coupled through the Coulomb interaction (no current flows between devices) have been proposed by the authors elsewhere.[4–6] We call such architectures quantum cellular automata (QCA). The QCA contains an array of quantum-dot cells that are connected locally by the interactions of the electrons contained within them. The quantum state of each multidot cell encodes the "logical" state of that cell. For this reason, each cell should ideally have exactly two stable states, since this will allow direct encoding of binary information.[7] Such two-state cells also need to exhibit bistable saturation to ensure that noise or small geometric variations do not overwhelm the signal.

To function as a CA, the state of each cell should be dependent on the states of its neighbors. In this paper, we compare the cell–cell coupling and bistable saturation of several different quantum cell designs that might form the basis of quantum cellular automata. All these designs have certain characteristics in common: a few (typically four or five) quantum dots connected by coupling coefficients and populated by a total of one to three electrons. In these cells the required interaction between neighbors is caused by the mutual Coulombic repulsion of the electrons contained in the cells. We use a very simple model of each cell, neglecting details relating to exactly how the quantum dot structures are realized, but focusing on the charge distribution among the dots and the Coulomb coupling between cells. We define a cell–cell response function that characterizes the interaction between neighboring cells.

In the next section we will introduce the theoretical model of the "standard cell," on which much of the work of Refs. 4–6 is based. It is the most thoroughly investigated cell design because it displays strong bistable saturation. We discuss the model Hamiltonian used for the cell, the method used to calculate the cell–cell response function, and the effects of nonzero temperature. In Sec. III we compare various other cell designs. Among these are different geometric arrangements of the quantum dots, one and three electron cells, and continuous quantum dashes. In Sec. IV, we extend our results to include the effects of multiple neighbors on a cell. We show that such effects in a system with three nearest neighbors can be thought of as majority voting logic. We show how this behavior can be used to implement programmable logic gates, and then show other possible implementations for dedicated AND and OR gates. A discussion and conclusion follow in Sec. V.

II. A MODEL QUANTUM CELL

The model "standard cell" design, shown schematically in Fig. 1(a), consists of five quantum dots located at the corners and the center of a square. Tunneling occurs between the central site and all four of the outer sites (near-neighbor tunneling), and to a lesser degree between neighboring outer sites (next-near-neighbor tunneling). It is assumed that the potential barriers between cells are high enough to completely suppress intercellular tunneling.

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Bistable saturation due to single electron charging in rings of tunnel junctions

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The behavior of rings of four small-capacitance tunnel junctions that are charged with two extra electrons is examined. Single electron charging effects result in quantization of charge on the metal electrode islands. To minimize the total electrostatic energy, the electrons localize on opposite electrodes, leading to a charge alignment in one of two configurations. We consider such rings as cells that may be capacitively coupled to each other in a cellular automaton architecture. The interaction between cells results in strong bistable saturation in the cell's charge alignment which may be used to encode binary information. Lines of such cells can be viewed as binary wires.

I. INTRODUCTION

Several schemes have been proposed for using Coulomb effects in small metal tunnel junctions to produce potentially useful behavior.[1,2] These have primarily exploited the Coulomb blockade of a tunneling current to produce single electron transistor action. The behavior of one- and two-dimensional arrays of small-capacitance tunnel junctions has also received considerable attention.[3]

Recently, we have theoretically examined the behavior of few-electron systems composed of quantum dots such as are usually fabricated in semiconductor heterostructures. We have shown bistable saturation in the charge alignment within quantum-dot cells that are Coulombically coupled to neighboring cells. This bistable interaction has formed the basis of a new architecture, termed quantum cellular automata (QCA).[4–7] Within the framework of this architecture, we have performed quantum simulations of designs for implementing binary wires, programmable logic gates, coplanar wire crossings, and circuits as complex as full adders.[8] The key advantages of the architecture are (1) only coupling between neighboring cells is necessary and this coupling is provided by the Coulomb interaction, (2) no power needs to be supplied to cells except at the edges of the array, (3) the design is robust in that it is insensitive to variations in physical parameters from cell to cell, and (4) as devices are reduced in dimension, the performance improves.

We examine here the behavior of cells composed of rings of metallic tunnel junctions with very small capacitance. The behavior of the rings is dominated by Coulomb exclusion effects.[9] We demonstrate that cells formed from these metal capacitors have the requisite bistable saturation and near-neighbor coupling behavior needed to provide the basis for an alternative implementation of the QCA architecture. The cell described here differs from those described elsewhere[4–8] in two fundamental ways. First, the cell is fabricated from small metal "islands" rather than from depleted two-dimensional electron gas and therefore contains many conduction electrons. Second, the coupling between islands and between cells is capacitive rather than simply Coulombic–the relevant Hamiltonian contains the capacitance matrix for the metallic array. This capacitive coupling is more amenable to control and design than the bare Coulomb interaction used in semiconductor implementation.

II. MODEL

We consider a cell consisting of four metal electrodes with small-capacitance tunnel junctions between them arranged in a ring, as shown schematically in Fig. 1(a). Each cell is occupied by two *extra* electrons supplied by the grounded substrate. The two electrons tend to occupy antipodal electrodes in the cell due to their mutual Coulomb repulsion.[10] This results in a preferential alignment of cell charge along one of the two perpendicular cell axes, as shown in Fig. 1(b). We define a polarization P which measures the extent of this alignment. If the charge on electrode i is ρ_i, then the polarization is defined as

$$P \equiv \frac{(\rho_1+\rho_3)-(\rho_2+\rho_4)}{\rho_1+\rho_2+\rho_3+\rho_4}. \tag{1}$$

If the extra electrons are completely localized on electrodes 1 and 3, the polarization is $+1$; if they are localized on electrodes 2 and 4, the polarization is -1. The presence of tunneling between electrodes means that the number of electrons on a metal electrode is not necessarily a good quantum number (it is a good quantum number in the limit of very little tunneling), so the ρ_i's need not be integers. Neighboring cells are capacitively coupled but no tunneling occurs between them.

The Hamiltonian[11] that describes the extra electrons in a cell labelled k can be written as follows:

$$H^k = \frac{1}{2}\sum_{i,j\in \text{cell } k} e^2(\mathbf{C}^{-1})_{i,j}\hat{n}_i\hat{n}_j + \sum_{\substack{i\in \text{cell } k \\ j\notin \text{cell } k}} e^2(\mathbf{C}^{-1})_{i,j}\hat{n}_i\hat{n}_j + \sum_{\substack{i,j\in \text{cell } k \\ i>j}} t_{i,j}(a_i^\dagger a_j + a_j^\dagger a_i). \tag{2}$$

Here $\mathbf{C}$ is the capacitance matrix describing the cell and the conductors surrounding it. The operators $a_i^\dagger$ and a_i create

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Logical devices implemented using quantum cellular automata

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We examine the possible implementation of logic devices using coupled quantum dot cells. Each quantum cell contains two electrons which interact Coulombically with neighboring cells. The charge distribution in each cell tends to align along one of two perpendicular axes, which allows the encoding of binary information using the state of the cell. The state of each cell is affected in a very nonlinear way by the states of its neighbors. A line of these cells can be used to transmit binary information. We use these cells to design inverters, programmable logic gates, dedicated AND and OR gates, and non-interfering wire crossings. Complex arrays are simulated which implement the exclusive-OR function and a single-bit full adder.

I. INTRODUCTION

Devices based on quantum-mechanical principles hold the promise of faster speeds and greatly reduced sizes. Most quantum device designs examined have been similar to classical device implementations in that they use currents and voltages to encode information. Thus although the device operations proposed have been based on quantum physics, the architectures have been conventional.

Employing quantum structures in conventional architectures has proven problematic for reasons directly related to the inherently small size of quantum-effect devices. The output signal of such ultrasmall devices, which is typically nanoamperes of current, must be able to drive several other similar devices, which may require a change of many millivolts in their input voltages. Another significant problem is that the capacitance of interconnecting wires tends to dominate the device behavior.[1] The wiring problem is aggravated by the fact that energy must be supplied to each computational element through power connections.

We have recently proposed a scheme in which Coulomb-coupled quantum devices are connected in a cellular automata architecture.[2] We call such architectures quantum cellular automata (QCA).[3–6] A QCA consists of an array of quantum-dot cells connected locally by the interactions of the electrons contained in each cell. The scheme is non-conventional in that the quantum state of each cell is used to encode binary information. The Coulomb interaction connects the state of one cell to the state of its neighbors. Thus the problems associated with small output currents and parasitic capacitances of connecting wires do not occur. "Binary wires" composed of linear arrays of cells are effective in transmitting information, coded in the cell states, from one place to another.[5]

In this paper we present simulations of QCA arrays, some of which are quite large, performing complex computational tasks. We review the basic cell operation and the use of linear arrays as a binary wire. Novel programmable logical gates and inverters are simulated and provide the basis for computing in this scheme. We demonstrate that it is possible to cross two QCA binary wires in the plane, with no interference. Building up more complicated operations from the basic gates, we simulate QCA implementations of an exclusive-OR function and a full adder. This serves to demonstrate that the interactions between cells are sufficiently local that hierarchical design is possible.

The calculations presented here are for zero temperature and assume the several-electron system has relaxed to its ground state before a valid output is read. Unlike conventional digital devices, the QCA operates on the principle that inelastic processes will always tend to drive the system back to its ground state.[7] The time evolution of the many-electron state of the system will in general be very complicated, but only the final ground-state properties are used for computing. Applying a new set of inputs places the system in an excited state. While the system is relaxing (presumably through a complicated process of exchanging energy with its environment), the outputs are not valid. Once the system has settled into its new ground state, the results of the calculation appear encoded in the states of the output cells located at an edge of the array. This idea of "computing with the ground state" is discussed at length in Ref. 4.

In the next section, we will give a review of QCA theory and the operation of the "standard cell." The standard cell is the most thoroughly studied cell design because it combines physically reasonable design parameters with excellent bistable saturation. A detailed treatment of the cell, various related cell designs, and our self-consistent calculations for arrays of coupled cells can be found in Refs. 3–6. Section II D discussed how lines of cells can be used to transmit information using a QCA binary wire. Section III shows a design for an inverter, and Sec. IV deals with the influence of several neighboring cells on the cell states. This leads to the idea of the majority voting logic gate and we demonstrate how its behavior can be used to implement a programmable AND/OR gate. Section V demonstrates a noninterfering planar crossing of two QCA wires. Section VI shows how these various ideas can be combined to form an exclusive-OR and a full adder.

II. COUPLED QUANTUM CELLS

The standard cell design, shown schematically in Fig. 1(a), consists of five quantum dots located at the corners and the center of a square. The cell is occupied by a total

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Coupled finite element/boundary element method for semiconductor quantum devices with exposed surfaces

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We present a study of the boundary conditions for the potential at exposed semiconductor surfaces in split-gate structures, which views the exposed surface as the interface between the semiconductor and air. A two-dimensional numerical algorithm is presented for the coupling between the nonlinear Poisson equation in the semiconductor (finite element method) and Laplace's equation in the dielectric (boundary element method). The utility of the coupling method is demonstrated by simulating the potential distribution in an *n*-type AlGaAs/GaAs split-gate quantum wire structure within a semiclassical Thomas–Fermi charge model. We also present a comparison of our technique to more conventional Dirichlet and Neumann boundary conditions.

I. INTRODUCTION

Recent advances in nanostructure fabrication have made it possible to realize semiconductor quantum devices by further confining a two-dimensional layer of electrons into wires or dots in which quantum effects are significant.[1,2] Typically, such device structures are defined by metallic split gates as schematically depicted in Fig. 1. In order to understand the potential distribution in these structures, one has to solve the Poisson equation in the two-dimensional problem domain,

$$\epsilon\nabla^2\phi = -\rho. \tag{1}$$

Here, ϕ is the confining electrostatic potential, ϵ is the dielectric constant of the respective material, and ρ is the charge density, which may depend upon the potential and for which different charge models have been developed.[3] Since Eq. (1) is a boundary value problem, one needs to know the values of the potentials and/or fluxes at the various boundaries. In particular at the exposed semiconductor surface, it has proven difficult to formulate appropriate boundary conditions. This is a crucial problem, especially in nanostructures where the charge carriers reside close to the surface, and a different choice for the boundary condition at the exposed surface may result in a noticeable difference in the confining potential of the quantum device. Highly accurate models of the potential variation will be needed to realize recently proposed computing architectures for quantum devices, so-called quantum cellular automata, which consist of cells of coupled quantum dots which are occupied by only a few electrons.[4]

In recent numerical studies,[5–11] the potential variation in structures like the one shown in Fig. 1 has been treated as a boundary value problem on the semiconductor domain and various boundary conditions have been assumed on the exposed semiconductor surface. One common approach is to utilize a Dirichlet boundary condition which simulates surface Fermi-level pinning at a characteristic energy level in the band gap,[9–11]

$$\phi|_s = -\phi_{\text{pin}}. \tag{2}$$

This approximation leads to an unrealistic discontinuous step in the potential energy at the edge of the biased gate between the values of the applied gate potential and the Fermi-level pinning. Another commonly used approach is to employ a Neumann boundary condition where one assumes a certain value for the outward normal electric field on the exposed semiconductor surface,[5,6]

$$\epsilon_s \left.\frac{\partial\phi}{\partial\mathbf{n}}\right|_s = Q_{\text{int}}. \tag{3}$$

$\mathbf{n}$ is the outward normal unit vector of the boundary, ϵ_s is the dielectric constant of the semiconductor, and Q_{int} is the charge density on the exposed surface. It can be shown that this approximation is only valid if the exposed semiconductor surface is large and smooth.[12] In typical split-gate structures used for quantum devices, the confined electron gas is very close to the exposed semiconductor surface and the separation between the split gates is rather small. The validity of the above two boundary conditions, thus, appears doubtful.

In this paper, we adopt an alternative viewpoint and develop an algorithm for its implementation: We view as the natural problem domain the semiconductor *and* the dielectric, as schematically shown in Fig. 2. Thus the artificial boundary conditions at the exposed semiconductor surface are replaced by more physical matching conditions at the interface between the semiconductor and dielectric. We assume that the potential ϕ is continuous across this interface and that the jump in the normal electric flux density is equal to the interface charge density,

$$\phi|_s = \phi|_d, \tag{4}$$

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